Level statistics and energy diffusion of XXZ spin chains(2) Equilibrium and nonequilibrium statistical mechanics in systems showing chaos and quantum chaos, Chaos and Nonlinear Dynamics in Quantum-Mechanical and Macroscopic Systems)

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Level statistics and energy diffusion of XXZ spin chains
量子XXZスピン鎖の準位統計とエネルギー拡散

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Abstract

次近接相互作用を含む量子 XXZ スピン鎖の準位統計とエネルギー拡散について議論する。扱う模型は、フラストレーションのある、有限なスピン 1/2 の XXZ 鎖である。非可積分の模型なので、準位統計は GOE を示す。この模型に振動磁場を印加した場合のエネルギー拡散を調べると、拡散定数が磁場の大きさと振動数に関してベキ乗則に従うことが分かる。そのベキ指数は、線形応答領域と非摂動領域では異なる。また、それらの領域の幅は、フラストレーションの強さに依存する。

There exists an accumulation of studies on quantum dynamics of classically chaotic systems. However, most of the systems treated so far are confined to those with a few degrees-of-freedom. Little study exists on deterministic quantum many-body systems exhibiting Gaussian orthogonal ensemble (GOE) spectral statistics, i.e. a hallmark of quantum chaos.

We discuss the statistical and dynamical properties of energy levels for XXZ spin chains, which are related to various important spin chains such as the Heisenberg chain and the Ising chain. We choose *frustrated* XXZ quantum spin chains with anti-ferromagnetic exchange interactions for the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) couplings. Advantage of the frustrated quantum systems is that we can expect quantum chaotic behavior appearing already in the low energy region near the ground state, which is important for real physics of condensed matter.

We give Hamiltonian for the NN and NNN coupled spin chain on L sites with a time-periodic oscillating magnetic field as

$$\begin{aligned} \mathcal{H}(t) &= J_1 \sum_{j=1}^{L} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + J_2 \sum_{j=1}^{L} (S_j^x S_{j+2}^x + S_j^y S_{j+2}^y + \Delta S_j^z S_{j+2}^z) \\ &- \sum_{j=1}^{L} S_j^z B_0 \sin\left(\omega t - \frac{2\pi j}{L}\right). \end{aligned} \tag{1}$$

Here, $S_j^\alpha = (1/2)\sigma_j^\alpha$ and $(\sigma_j^x, \sigma_j^y, \sigma_j^z)$ are the Pauli matrices on the jth site; the periodic boundary conditions (P. B. C.) are imposed. The period of Eq. (1) is $T = 2\pi/\omega$. Because of the coexisting spatial P. B. C., however, the effective period of the adiabatic energy spectra is given by $T' = T/L = (2\pi/\omega)/L$. In other words, the period of the Hamiltonian operator is T, and the spectral flow of the eigenvalues has the effective period T'. This periodicity property comes from the traveling wave form of Eq. (1).

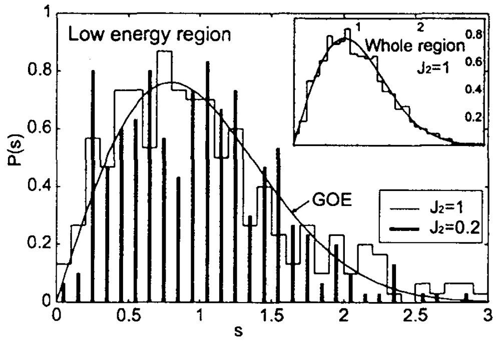

Fig. 1: Level-spacing distribution at $t = \pi/4$ for lowest 300 levels from the ground state (about 10% of all 3003 levels); $L = 14$, $\Delta = 0.3$, $B_0 = 0.8$ [2].

When we investigate level statistics, we desymmetrize the Hamiltonian and use the unfolded eigenvalues to find universal properties of the energy levels. When we investigate energy diffusion for the model, Eq. (1), we also desymmetrize the Hamiltonian. Then, to see universal properties of the energy diffusion, we scale the Hamiltonian so that the full range of adiabatic energy eigenvalues becomes almost free from from these parameters. We define the scaled Hamiltonian $H(t)$ so that the full energy range equals L at $t = 0$. The time-dependent Schrödinger equation is then given by

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle. \tag{2}$$

The solution of Eq. (2) consists of a sequence of the infinitesimal processes as

$$|\psi(t)\rangle = U(t; t-\Delta t)\, U(t-\Delta t; t-2\Delta t) \ldots U(2\Delta t; \Delta t)\, U(\Delta t; 0)|\psi(0)\rangle. \tag{3}$$

The initial state $|\psi(0)\rangle$ is taken to be the ground state. To calculate a time evolution operator $U(t+\Delta t; t)$, we use the fourth-order decomposition formula for the exponential operator.

Level statistics for the model shows GOE behavior for $J_2 \neq 0$, while Poisson-like behavior appears for $J_2 \simeq 0$ or $\Delta \simeq 1$ because of some finite-size effects [1]. Incidentally, the characteristic behavior of level statistics does not depend on the energy range. As shown in Fig. 1, GOE level statistics is observed in the low energy region.

To investigate time evolution of energy diffusion, we evaluate energy variances at each integer multiple of the effective period $T' = T/L = (2\pi/\omega)/L$. The energy variance of our concern is *the variance around the ground state energy* E_0 and is defined by

$$\delta E(t)^2 = \langle\psi(t)|[H(t) - E_0]^2|\psi(t)\rangle. \tag{4}$$

Time evolution of $\delta E(t)^2$ is shown in Fig. 2. Figure 2 shows the normal diffusion in energy space, i.e. a linear growth of $\delta E(t)^2$ in time, during the first period. The energy variances will finally saturate because the system size we consider is finite. On the other hand, the energy variances can also saturate because of another reason, i.e. the dynamical localization effect. It is associated with a periodic perturbation. In any case, diffusion coefficients have to be determined for times where saturation does not yet occur. We determine the diffusion coefficient D from the fitting

$$\delta E(t)^2 = Dt + \text{const}. \tag{5}$$

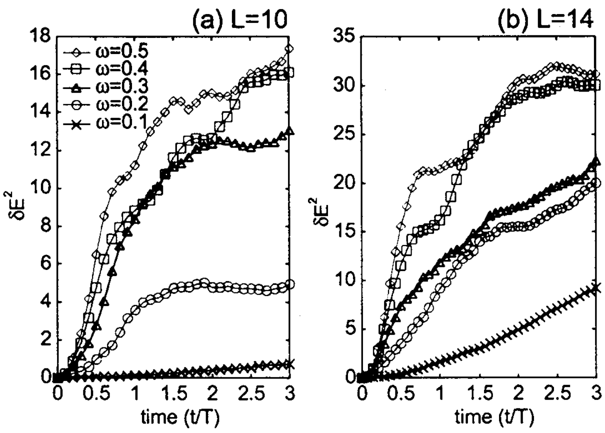

Fig. 2: Time evolution of energy diffusion for (a) $L = 10$ and (b) $L = 14$ [2]. The parameters are the following: $J_1 = J_2 = 1.0$, $\Delta = 0.3$, $B_0 = 1.0$.

to some data points around the largest slope in the first period, where the normal diffusion is expected.

Now we consider two parameter regimes to analyze parameter dependence of diffusion coefficients. So long as the changing rate $\dot{X}$ of a perturbation parameter is not very large, the diffusion coefficient can be calculated using the Kubo formula. We call such a parameter regime "linear response" regime. In the linear response regime, $D \propto \dot{X}^2$ (See, e.g. Ref. [3]). When $\dot{X}$ is large, however, the perturbation theory fails. We call such a parameter regime "non-perturbative" regime. In the non-perturbative regime, the diffusion coefficient is smaller than that predicted by the Kubo formula [3, 4]. According to Ref. [3], $D \propto \dot{X}^{\gamma}$ with $\gamma \leq 1$ in the non-perturbative regime. We note that $\dot{X} \propto B_0\omega$ in this paper. Both Refs. [3] and [4] are based on the random matrix models, which are utterly different from our deterministic one. Here we do not consider a near-adiabatic regime. Because of large energy gaps around the ground state, this regime cannot result in the notable energy diffusion.

Figure 3 shows how the behavior of D changes between a linear response regime and a non-perturbative regime. The diffusion coefficient D obeys the power law $D \propto (B_0\omega)^{\beta}$ with its power $\beta = 2$ in the linear response regime and $\beta = 1$ in the non-perturbative regime. For small $B_0\omega$, the power law seems to fail because of some finite-size effects. These universal feature is confirmed also for $L = 14$ [2]. Actually, D obeys the power law better for $L = 14$ than $L = 10$. In addition, error bars are shorter for $L = 14$ than $L = 10$. Here, we have used the data of $\omega \leq 1$. We cannot expect meaningful results in a large-ω regime since energy diffusion is not normal there. In fact, for a large-ω regime, the increase of energy variances per effective period hardly depend on ω before the time when $\delta E(t)^2$ starts to decrease.

Figure 3 suggests that the strength of frustration should affect the range of the linear response regime. The range of the linear response regime is shorter for $J_2 = 0.2$ than for $J_2 = 1.0$, while that of the non-perturbative regime is larger for $J_2 = 0.2$ than for $J_2 = 1.0$. In fact, when $J_2 = 0$ (i.e. the integrable case), $D \propto (B_0\omega)^{\beta}$ with $\beta = 1$ for almost all the data in the same range of $B_0\omega$ as that of Fig. 3.

In conclusion, we have explored the energy diffusion from the ground state in frustrated

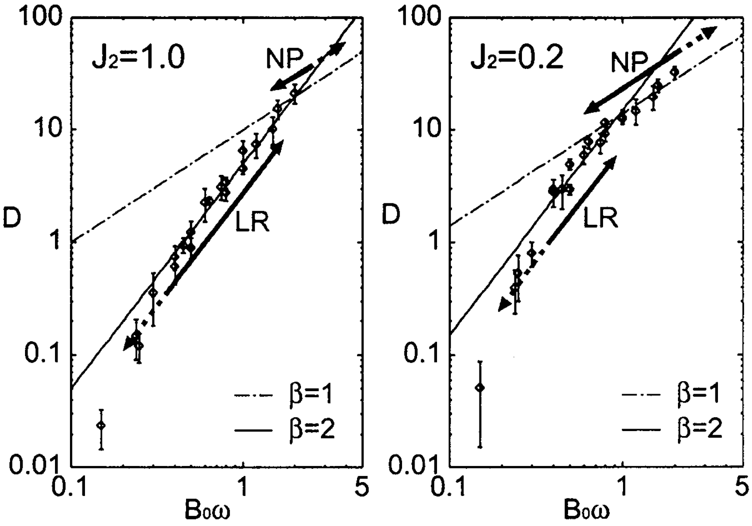

Fig. 3: Dependence of the diffusion coefficients on $B_0\omega$ for $L = 10$ [2]. The chained line and the solid line are just eye guides for $D \propto (B_0\omega)^\beta$ with $\beta = 1$ and $\beta = 2$, respectively. LP and NP are short for Linear response regime and Non-perturbative regime, respectively.

quantum XXZ spin chains, which exhibit GOE spectral statistics already in the low energy region near the ground state. Diffusion coefficients D obey the power law with respect to both the field strength and driving frequency with its power being two in the linear response regime and equal to unity in the non-perturbative regime. The ranges of the linear response regime and the non-perturbative regime depend on the strength of frustration, i.e. J_2. On the other hand, the characteristic behavior of level statistics does not depend on J_2 except for the case of $J_2 \simeq 0$. The energy diffusion reveals generic features of the frustrated quantum spin chains, which cannot be captured by the analysis of level statistics.

Acknowledgements

The author would like to thank T. Deguchi and K. Nakamura for collaboration. The present study was partially supported by Hayashi Memorial Foundation for Female Natural Scientists.

Reference

[1] K. Kudo and T. Deguchi, cond-mat/0409761.

[2] K. Kudo and K. Nakamura, in preparation

[3] M. Wilkinson and E. J. Austin, J. Phys. A **28** (1995), 2277; Phys. Rev. A **46** (1992), 64.

[4] D. Cohen and T. Kottos, Phys. Rev. Lett. **85** (2000), 4839.